Amendments to the Claims

This listing of claims will replace all prior versions, and listings, of claims in the application:

Listing of Claims

1. (Currently Amended) A method for selecting at least one lead-candidate compound capable of binding as a ligand to a protein from a database of trial compounds comprising information on atomic types, covalent bonds and three-dimensional structures of compounds in the database, comprising:

a) inputting at least one query molecule that is known to bind, or expected to be capable of binding, to a three-dimensional structure of the protein;

b) screening lead-candidate compounds from the compound database by matching modes of covalent bonds between the query molecule and the trial compounds stored in the database and judging similarity of partial structures of the query molecule and the trial compounds based on two-dimensional graphs of the query molecule and the trial compounds where each atom is represented as a node and each covalent bond is represented as an arc;

c) estimating a binding scheme of the lead-candidate compounds to the three-dimensional structure of the protein based on three-dimensional information of the query molecule, binding scheme of the query molecule to the three-dimensional structure of the protein, and correspondence of the mode of covalent bonds of the partial structures of the query molecule and the trial compounds; and

d) outputting at least one lead-candidate compound capable of binding to the protein to a display or a user.

2-5. (Canceled)

6. (Previously Presented) The method of claim 1, which further comprises:

calculating one or more parameters relating to interaction between the lead-candidate compounds and the protein; and

screening the lead-candidate compounds capable of binding as a ligand to the protein based on the parameters relating to interaction between the lead-candidate compounds and the protein.

7-10. (Canceled)

11. (Previously Presented) The method of claim 1, wherein step (a) further comprises constructing the structure of the at least one query molecule by an automatic structure construction method.

12-14. (Canceled)